Problem Set 7

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1)

$$\psi(x) = \begin{cases} 2\sqrt{a^3}xe^{-ax} \text{ if } x > 0\\ 0 \text{ if } x < 0 \end{cases}$$

1.a)

$$\int_0^\infty |\psi(x)|^2 dx = \int_0^\infty \left| 2\sqrt{a^3} x e^{-ax} \right|^2 dx$$
$$= \int_0^\infty 4a^3 x^2 e^{-2ax} dx$$
$$= 4a^3 \int_0^\infty x^2 e^{-2ax} dx$$
$$= 4a^3 \cdot \frac{1}{4a^3}$$
$$= 1$$

So yes, it is normalized!

1.b)

We can set $\frac{d}{dx} |\psi(x)|^2 = 0$ to find the maximum of the function. We know that as $x \to \infty$, $e^{-2ax} \to 0$, so we do not need to worry about maximums at the bounds.

$$\frac{\mathrm{d}}{\mathrm{d}x} |\psi(x)|^2 = \frac{\mathrm{d}}{\mathrm{d}x} 4a^3 x^2 e^{-2ax}$$

$$= e^{-2ax} (2x - 2ax^2)$$

$$0 = e^{-2ax} (2x - 2ax^2)$$

$$0 = 2x - 2ax^2$$

$$2x = 2ax^2$$

$$x \neq 0 \Longrightarrow x = \frac{1}{a}$$

Therefore, the maximum of the function is at $x = \frac{1}{a}$.

1.c)

$$\int_0^{\frac{1}{a}} |\psi(x)|^2 dx = \int_0^{\frac{1}{a}} \left| 2\sqrt{a^3} x e^{-ax} \right|^2 dx$$
$$= \int_0^{\frac{1}{a}} 4a^3 x^2 e^{-2ax} dx$$
$$= 1 - \frac{5}{e^2}$$
$$= 0.323$$

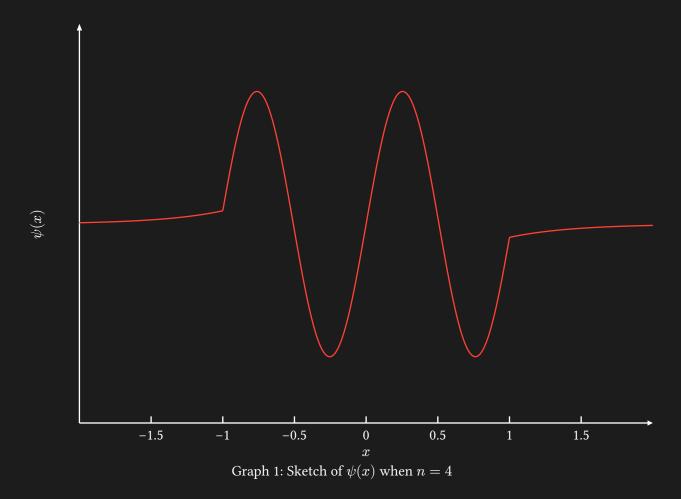
2)

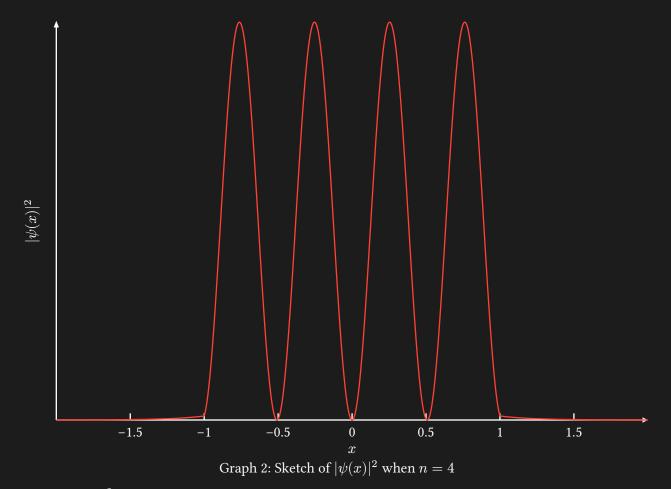
We can plot the wave function. We know that it needs to have 3 nodes and be an odd function because n=4.

To make this plot, I chose values for k and K until the plot looked *nice*, which is definitely not the *numerical* way of doing things (but this is just a sketch).

```
def psi(x):
    a = 1
    k = 2 * np.pi - 0.1
    K = 2.3

if x < -a:
    return np.exp(K * x)
elif -a <= x <= a:
    return np.sin(k * x)
else:
    return -np.exp(-K * x)</pre>
```





To get $|\psi(x)|^2$, we just need to square each value in $\psi(x)$ because it is a real function. We can see the small amount of "leakage" into the classically forbidden region.

3)
$$U(x) = \begin{cases} 0 & \text{if } |x| > a \\ -U_0 & \text{if } |x| < a \end{cases}$$

3.a)
$$E_1 = -\frac{1}{2}U_0$$

We know that the first excited state will use an odd function as there will be one node in $\psi(x)$. Let's define the following quantities:

$$k = \sqrt{\frac{2m}{\hbar^2}(U_0 - |E|)}$$

$$K = \sqrt{\frac{2m|E|}{\hbar^2}}$$

We can plug in $E_1=-\frac{1}{2}U_0$ into these equations.

$$k = \sqrt{\frac{2m}{\hbar^2} \left(\frac{1}{2}U_0\right)}$$

$$= \sqrt{\frac{mU_0}{\hbar^2}}$$

$$K = \sqrt{\frac{2m(\frac{1}{2}U_0)}{\hbar^2}}$$

$$= \sqrt{\frac{mU_0}{\hbar^2}}$$

We know that $K=-k\cot(ka)$, which then shows that:

$$\begin{split} \sqrt{\frac{mU_0}{\hbar^2}} &= -\sqrt{\frac{mU_0}{\hbar^2}}\cot\left(\sqrt{\frac{mU_0}{\hbar^2}}a\right) \\ -1 &= \cot\left(\sqrt{\frac{mU_0}{\hbar^2}}a\right) \\ &\operatorname{arccot}(-1) &= \sqrt{\frac{mU_0}{\hbar^2}}a \\ &\operatorname{arccot}^2(-1)\frac{\hbar^2}{ma^2} &= U_0 \end{split}$$

In order for cotan to be -1, $ka = \frac{3\pi}{4}$. We are in first excited state, so we know that $ka = \frac{3\pi}{4}$ and not some integer multiple of this value.

$$k = K = \frac{3\pi}{4a}$$

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x$$

$$= A^2 \left[\underbrace{\int_{-\infty}^{-a} e^{2Kx} \, \mathrm{d}x}_{\text{region I}} + \underbrace{\int_{-a}^{a} \frac{e^{-2Ka}}{\sin^2(ka)} \sin^2(kx) \, \mathrm{d}x}_{\text{region III}} + \underbrace{\int_{a}^{\infty} e^{-2Kx} \, \mathrm{d}x}_{\text{region III}} \right]$$

For region I, we have the following:

$$\int_{-\infty}^{-a} e^{2Kx} dx = \frac{1}{2K} e^{2Kx} \Big|_{x=-\infty}^{-a}$$
$$= \frac{e^{-2Ka}}{2K}$$

For region 3, we have something very similar:

$$\int_{a}^{\infty} e^{-2Kx} dx = -\frac{1}{2K} e^{-2Kx} \Big|_{x=a}^{\infty}$$
$$= \frac{e^{-2Ka}}{2K}$$

Region 2 is the following. We will ignore the coefficients for now...

$$\begin{split} \int_{-a}^{a} \sin^{2}(kx) \, \mathrm{d}x &= \frac{1}{2} \int_{-a}^{a} [1 - \cos(2kx)] \, \mathrm{d}x \\ &= \frac{1}{2} \left[x - \frac{\sin(2kx)}{2k} \right] \Big|_{x = -a}^{a} \\ &= \frac{1}{2} \left[2a - \frac{\sin(2ka)}{k} \right] \\ &= a - \frac{\sin(2ka)}{2k} \end{split}$$

Adding back in the coefficients for region II:

$$\frac{e^{-2Ka}}{\sin^2(ka)} \left(a - \frac{\sin(2ka)}{2k} \right)$$

Now, we need to solve for A:

$$1 = A^{2} \left[\frac{e^{-2Ka}}{2K} + \frac{e^{-2Ka}}{2K} + \frac{e^{-2Ka}}{\sin^{2}(ka)} \left(a - \frac{\sin(2ka)}{2k} \right) \right]$$

$$= A^{2} \left[e^{-2Ka} \left(\frac{1}{K} + \frac{1}{\sin^{2}(ka)} \left(a - \frac{\sin(2ka)}{2k} \right) \right) \right]$$

$$\implies A = \left[e^{-2Ka} \left(\frac{1}{K} + \frac{1}{\sin^{2}(ka)} \left(a - \frac{\sin(2ka)}{2k} \right) \right) \right]^{-\frac{1}{2}}$$

$$= e^{Ka} \left[\left(\frac{1}{K} + \frac{1}{\sin^{2}(ka)} \left(a - \frac{\sin(2ka)}{2k} \right) \right) \right]^{-\frac{1}{2}}$$

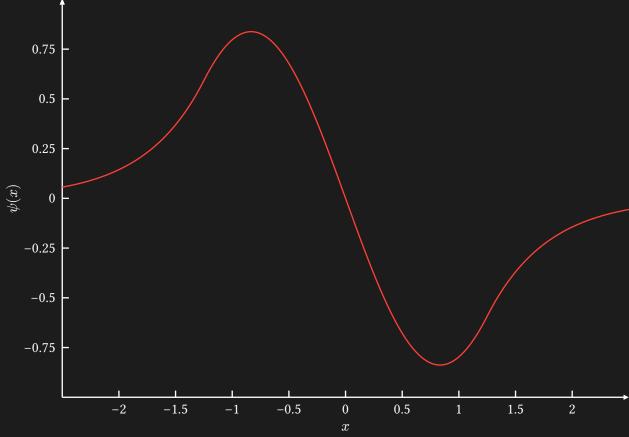
We can simplify this as we know $k = K = \frac{3\pi}{4a}$.

$$A = e^{\frac{3\pi}{4}} \left[\frac{4a}{3\pi} + \frac{1}{\sin^2(3\frac{\pi}{4})} \left(a - \frac{\sin(3\frac{\pi}{2})}{\frac{3\pi}{2a}} \right) \right]^{-\frac{1}{2}}$$

$$= e^{\frac{3\pi}{4}} \left[\frac{4a}{3\pi} + 2\left(a + \frac{2a}{3\pi} \right) \right]^{-\frac{1}{2}}$$

$$= \frac{e^{3\frac{\pi}{4}}}{\sqrt{\frac{2a}{3\pi}(4+3\pi)}}$$

$$\psi(x) = \begin{cases} e^{\frac{3\pi}{4}} \left(\frac{8a}{3\pi} + 2a\right)^{-\frac{1}{2}} e^{\frac{3\pi}{4a}x} & \text{if } x < -a \\ \frac{-1}{\sqrt{\frac{4a}{3\pi} + a}} \sin\left(\frac{3\pi}{4a}x\right) & \text{if } -a \le x \le a \\ -e^{\frac{3\pi}{4}} \left(\frac{8a}{3\pi} + 2a\right)^{-\frac{1}{2}} e^{-\frac{3\pi}{4a}x} & \text{if } x > a \end{cases}$$



Graph 3: Plot of $\psi(x)$ as shown above

3.c)

We can first solve for the probability of being on one side of the forbidden zones, and then double that to get the probability of being in either forbidden zone.

$$A^{2} \int_{a}^{\infty} e^{-2Kx} dx = \frac{A^{2}}{-2K} [e^{-2Kx}] \Big|_{x=a}^{\infty}$$

$$= \frac{A^{2}}{2K} e^{-2Ka}$$
plug in for $K \Longrightarrow = \frac{2A^{2}a}{3\pi} e^{-\frac{3}{2}\pi}$
plug in for $A \Longrightarrow = \frac{e^{\frac{3}{2}\pi - \frac{3}{2}\pi} \cdot 2a}{\frac{2a(4+3\pi)}{(3\pi)} \cdot 3\pi}$

$$= \frac{1}{4+3\pi}$$

$$\approx 0.07449$$

This is only half of the probability, so we can double it to find the probability that the particle is in the forbidden region.

$$P(\text{particle in forbidden region}) = \frac{2}{4 + 3\pi}$$

$$\approx 0.149$$

This is suprisingly large, considering that classically it would impossible for the particle to be observed in this region.

4)

$$\psi(x) = Axe^{-\frac{x^2}{L^2}}$$

We can plug this function into the Schroedinger equation to find U(x).

$$\begin{split} \frac{\mathrm{d}}{\mathrm{d}x}\psi(x) &= Ae^{-\frac{x^2}{L^2}} \left(\frac{-2x^2}{L^2}\right) + Ae^{-\frac{x^2}{L^2}} \\ &= \frac{\psi(x)}{x} \left(1 - \frac{2x^2}{L^2}\right) \\ \frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) &= \frac{\mathrm{d}^2}{\mathrm{d}x^2} \frac{\psi(x)}{x} \left(1 - \frac{2x^2}{L^2}\right) \\ &= \frac{\psi(x)}{x} \left(1 - \frac{4x}{L^2}\right) + \left(1 - \frac{2x^2}{L^2}\right) \left(\frac{-2\psi(x)}{L^2}\right) \\ &= Ae^{-\frac{x^2}{L^2}} \left(-\frac{6}{L^2} + \frac{4x^2}{L^4}\right) \end{split}$$

We can (finally) plug this into the SE.

$$\begin{split} -\frac{2m}{\hbar^2}U(x)\psi(x) &= \psi(x)\Biggl(-\frac{6}{L^2} + \frac{4x^2}{L^4}\Biggr) \\ U(x) &= \frac{\hbar^2}{2mL^2}(4x^2 - 6) \end{split}$$

This is a parabola that opens upwards.

$$U(0) = \frac{-6\hbar^2}{2mL^2}$$

At x=0, the potential energy is $\frac{-3\hbar^2}{mL^2}$.